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# 1. Overview

The Chemical Science and Technology Laboratory (CSTL) of the National Institute of Standards and Technology (NIST) is the United States' reference laboratory for chemical measurements, entrusted with developing, maintaining, advancing, and enabling the chemical measurement system for the United States of America, thereby enhancing U.S. industry's productivity and competitiveness, assuring equity in trade, and improving public health, safety, and environmental quality. This year NIST celebrates its 100<sup>th</sup> anniversary; it is notable that the Chemistry Division was there from the start in 1901, recognizing the importance of chemical measurements and standards to our emerging industrial nation.

Today as part of the Commerce Department's Technology Administration, NIST's mission is to strengthen the U.S. economy and improve the quality of life by working with industry to develop and apply technology, measurement science, and standards. The vision that NIST has set for itself is to provide U.S. industry with the world's best technical infrastructure and return the best possible value to the economy and society. NIST provides scientific leadership for the Nation's measurement and standards infrastructure and ensures the availability of essential reference data and measurement capabilities. To discharge these responsibilities, NIST maintains expertise in a broad range of science and technology areas. The Chemical Science and Technology Laboratory is responsible for measurements, data, and standards in chemical, biochemical, and chemical engineering sciences. Building on a one hundred year history of technical excellence, today's CSTL has the most comprehensive array of chemical, physical, and engineering measurement capabilities of any group worldwide working in chemical science and technology.

As we enter into the third millennium, CSTL strives to be a world-class research laboratory that is recognized by the Nation as the primary source for the chemical, biochemical, and chemical engineering measurements, data, models, and reference standards required to enhance U.S. industrial competitiveness in the world market. This vision for CSTL will be achieved and the mission of CSTL implemented through pursuit of the following three goals.

**Measurement Standards:** Establish CSTL as the pinnacle of the national traceability and international comparability structure for measurements in chemistry, chemical engineering, and biotechnology, and provide the fundamental basis of the nation's measurement system. This objective is achieved by

- Developing and demonstrating international comparability for chemical and physical measurements.
- Supporting and strengthening the vertical traceability structure in the U.S., and
- Supporting and strengthening voluntary standards organizations.

**Chemical and Process Information:** Assure that U.S. industry has access to accurate and reliable data and predictive models to determine the chemical and physical properties of materials and processes. This objective is realized through

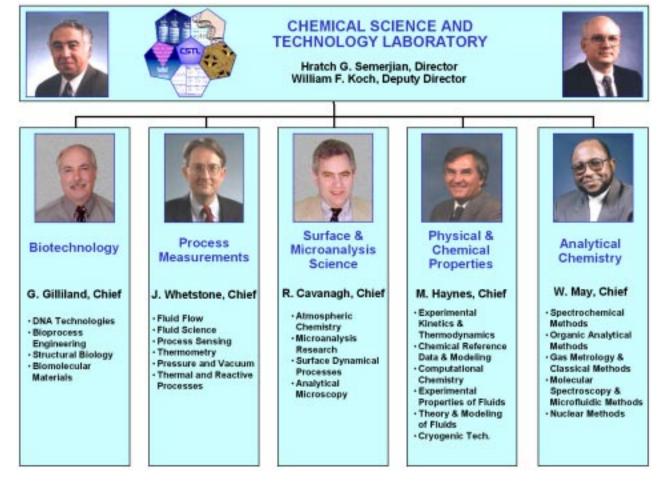
- Developing benchmark data for the properties of important substances, classes of substances, and systems;
- Developing data collections, data prediction methods, and models to meet high priority industrial and national needs:
- Contributing to the development of consensus standards for key properties, substances, and processes; and
- Developing procedures or protocols for data access, facilitating data exchange, and by disseminating properly formatted data.

**Measurement Science:** Anticipate and address next-generation measurement needs of the Nation. This final goal is achieved by

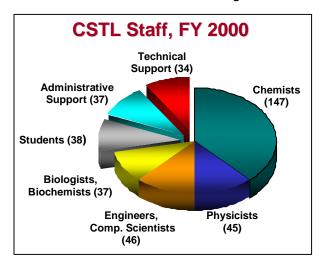
- Maintaining a strong and cutting-edge research program to support the Nation's measurement and standards infrastructure,
- Establishing new measurement capabilities to support new or advanced technology development and dissemination.

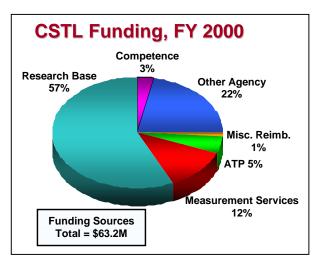
## Organizational Structure and Resources

CSTL is organized to reflect the technical expertise that is the foundation of our technical program and allows us to accomplish our mission. The Laboratory consists of five Divisions: Biotechnology Division, Process Measurements Division, Surface and Microanalysis Science Division, Physical and Chemical Properties Division, and Analytical Chemistry Division. Each Division employs a group structure organized to achieve synergy and critical mass in its technical program areas.



To achieve its goals, CSTL maintains an experienced, well-educated professional staff. The permanent staff numbered 269 in FY00, in addition to 115 temporary and part-time employees. Also, there were almost an equivalent number of guest researchers who work closely with CSTL staff in various aspects of the research program. The technical capabilities of CSTL staff are extensive. CSTL technical staff holds degrees in chemistry, physics, engineering, biology, geology, and computer science. A technical support staff augments the professional staff. Approximately 77% of the technical staff have PhD degrees.





CSTL's physical facilities are located at the major NIST sites in Gaithersburg, Maryland and Boulder, Colorado, as well as at the Center for Advanced Research in Biotechnology (CARB) in Rockville, Maryland and the Marine Environmental Health Research Laboratory (MEHRL) in



Charleston, South Carolina. The Physical and Chemical Properties Division has operations located at the NIST sites in Gaithersburg and Boulder. Biotechnology Division staff works closely with that of the University of Maryland Biotechnology Institute located at CARB. The Analytical Chemistry Division is the primary liaison with MEHRL, having staff located in Charleston. MEHRL is a cooperative research facility involving NIST, the National Oceanic and At-

mospheric Administration, the South Carolina Department of Natural Resources, the University of Charleston, and the Medical University of South Carolina.

The Analytical Chemistry and Biotechnology Divisions have completed their first full year in the Advanced Chemical Sciences Laboratory (ACSL), the first new research facility on the NIST Gaithersburg Campus in over thirty years. Although ACSL adds significantly to CSTL's research capabilities, it does not meet all facility needs of our program.



In the last few years NIST has developed a facilities master plan that envisions an additional facility, the Advanced Measurements Laboratory (AML), (specified to meet low vibration/high temperature stability needs), as well as renovations of the general-purpose laboratories. Con-



struction of the Advanced Measurements Laboratory (AML) on the Gaithersburg campus has begun with completion planned for 2004. This new facility will accommodate most of the Surface and Microanalysis Science Division, as well as the Pressure and Temperature activities in the Process Measurements Division and the laser diagnostic activities in the Physical and Chemical Properties Division.

#### Customers

CSTL is a multifaceted, synergistic organization with a unique customer base. Perhaps the most remarkable aspect of the CSTL customer-base is its breadth. The primary customers we serve are: industry; federal, state, and local government agencies; standards and industrial trade organizations; and the academic and scientific communities.

U.S. industry is the largest consumer of our products and services. These customers come from established industrial sectors, such as the chemical manufacturers, and emerging industries, such as biotechnology. The products and services they rely on are as varied as Standard Reference Materials. Standard Reference Data, calibration services, and novel measurement methods. Reference materials and calibrations provide traceability to the International System of Units (SI), which is essential to fair trade, improved reliability of measurements, and Data compilations regulatory compliance. modeling of chemical processes and rational product design. New measurement techniques ensure quality and improve efficiency, and in turn enhance competitiveness.

## Customer Segments

Automotive & Transportation
Biotechnology
Chemical Processors
Energy Systems
Food & Nutrition
Healthcare & Pharmaceuticals
Instrumentation
Metals & Materials
Microelectronics
National Security
Petrochemicals
Regulatory Agencies

Federal, state, and local governments are another important consumer of our products and services. These agencies use our products and services in ways similar to the commercial sector, but in different arenas. For example, calibrations, evaluated data, and reference materials are used to ensure the reliability of environmental monitoring programs. Carefully characterized physiological samples lend credibility to forensics tests. Measurement technologies developed and perfected in CSTL verify compliance with international treaties. Other national laboratories exploit the expertise and techniques developed here in discharging their mandates.

A final group that uses our expertise includes trade organizations, standards committees, and the academic and scientific community. These groups rely on CSTL's expertise for advice and guidance in establishing practical standards and uniform protocols. The academic and scientific communities rely on the data produced and complied by our staff as touchstones for their own research.

The needs of our customers are reflected significantly in our program priorities. Customers purchase our products and services, e.g., SRMs, Standard Reference Data, and calibration services, collaborate with us through consortia and Cooperative Research and Development Agreements (CRADAs), contract for our services, and interact through interlaboratory comparison exercises,

conferences, and workshops, and informally with our technical staff. Some of the CSTL outputs and interactions in FY2000 are summarized in the following table.

Selected CSTL Outputs - FY 2000										
Div.	Pubs.	Talks	Committees <sup>1</sup>	Seminars	Conferences	CRADAs	Patents Issued	SRMs /RMs <sup>2</sup>	SRDs	Cals. <sup>3</sup>
830	3	13	31	12	1	0	0	0	0	0
831	98	201	53	32	1	3	1	1	0	0
836	95	87	108	22	10	6	5	2	0	542
837	107	128	90	7	6	0	0	5	4	0
838	166	162	81	27	8	6	1	0	7	1
839	135	170	141	11	13	2	0	239	1	320
<b>Totals</b>	604	<b>761</b>	504	111	39	17	7	247	12	863

<sup>&</sup>lt;sup>1</sup> Committee totals include 36 editorships

### **Division Key:**

830	Laboratory Office	837	Surface and Microanalysis Science Division
831	Biotechnology Division	838	Physical and Chemical Properties Division
836	Process Measurements Division	839	Analytical Chemistry Division

SRM – Standard Reference Materials SRD – Standard Reference Data

## Program Planning, Assessment and Evolution

Keeping in mind its three goals (Measurement Standards, Chemical Information, and Measurement Science), CSTL sets its program priorities using criteria (see box) that emphasize the NIST/CSTL mission to work with U.S. industry to enhance U.S. economic growth. CSTL works proactively with its customers to anticipate the measurement and related infrastructural technology needs of U.S. industry. Identification of technological areas where new or improved measurements and standards are, or will be, needed allows CSTL to draw upon research in measurement science to develop metrology solutions supporting the needs of our customers. An additional criterion based on the utilization of newly developed scientific knowledge reflects CSTL's commitment to maintain-

## Setting Program Priorities

## Criteria:

- 1) the magnitude and immediacy of industry's need;
- 2) how well the activity matches the CSTL mission;
- 3) the degree to which CSTL involvement impacts success:
- 4) the size and nature of the impact;
- 5) whether CSTL can respond with an output of sufficiently high quality in a timely manner.

ing a strong measurement science research program as a vital resource for solutions to measurement challenges.

CSTL serves a growing list of needs from established customer industries, and must simultaneously work to assure the technical infrastructure for the industries of tomorrow. CSTL identifies industry's leading metrology needs and generates agreement on technical objectives by using conferences, workshops, direct technical exchange with industry, technology roadmapping exer-

<sup>&</sup>lt;sup>2</sup> SRMs/RMs includes 63 NTRMs<sup>®</sup> (NIST Traceable Reference Materials)

<sup>&</sup>lt;sup>3</sup> Calibrations were performed for over 345 customers



cises, and joint research through participation in consortia and CRADAs. In addition, CSTL uses technology assessments and economic impact analyses (see later section of this Report) in its strategic planning process. Through all these channels, industry input helps to set the direction and emphasis of CSTL programs. CSTL encourages individual companies and institutions to shape and participate in new

initiatives. CSTL also strives to anticipate metrology needs generated by new regulations by monitoring legislative developments and consulting with regulatory agencies.

CSTL balances its programs among development of essential measurement standards and technologies and basic research in measurement science to ensure a healthy science and infrastructural technology base for the future. Each Division in CSTL performs basic and applied research and maintains close contacts with the appropriate industrial and scientific communities to assess and anticipate the future measurement needs of its customer base. As part of its strategic planning process, in the fourth quarter of each fiscal year, CSTL assesses and prioritizes future needs and re-orients its research program to reflect the changing needs of its customer base. Areas are identified where new scientific or technological emphasis is required to meet emerging U.S. industry needs, or areas where the industrial need for products of existing programs is anticipated to increase significantly. Resources are redirected from activities where efforts have reached maturity and produced their anticipated results. Thrust areas where CSTL has re-oriented its program over the last several years include: national traceability and international comparability of measurements; computational chemistry; bioinformatics; chemical analysis at critical surfaces and interfaces: measurement methods and standards for next-generation health status markers: kinetics and thermodynamic data for industrial processes; tissue engineering; combinatorial techniques; clusters secondary ion mass spectrometry; and in vitro diagnostic device standards. For FY 2001 CSTL has expanded its efforts in the following areas: molectronics; high throughput screening; bioMEMS; dynamic data compilations; and genetically modified organisms.

These new thrust areas, along with on-going projects and activities, form the basis of CSTL's overall portfolio of programs. To define and articulate this portfolio (and basically to answer the question: "What does CSTL do?"), CSTL has aligned its activities along twelve programmatic themes. (See box at right.) The next twelve sections of this Report will delve into each of these programs individually, highlighting major activities and accomplishments in these areas for FY2000. Technical details of these activities can be found on CSTL's website <a href="http://www.cstl.nist.gov/">http://www.cstl.nist.gov/</a> or by contacting the principle investigators listed in the Report.

### CSTL's Twelve Programs

Chemical Characterization of Materials
Process Metrology
Chemical and Biochemical Sensing
Nanotechnology
Healthcare Measurements
Environmental Measurements
Microelectronics
Physical Property Data
Chemical and Biochemical Data
Bio-Molecules and Materials
DNA Technologies
International Measurement Standards

